# NIST Combinatorial Methods Center
# Informatics Workshop


## MatML: Definition, History, Results

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**22 May 2003**

# MatML: Definition

***MatML is an eXtensible Markup Language for the management and exchange of materials property data on the WWW.***

## Aluminum Alloy Data in HTML

```
<p>
1350<br>
metal<br>
aluminum alloy<br>
ASTM B230<br>
H18<br>
From “Properties of Aluminum Alloys - Tensile, Creep, and Fatigue Data at High and Low Temperatures.”<br>
Axial-Stress Fatigue Strength (ksi)<br>
<table>
<tr><td>23</td></tr>
<tr><td>17</td></tr>
<tr><td>15</td></tr>
</table>
```

## Aluminum Alloy Data in MatML

```
<MatML_Doc>
  <Material>
    <BulkDetails>
      <Name>1350</Name>
      <Class>metal</Class>
      <Subclass>aluminum alloy</Subclass>
      <Specification>ASTM B230</Specification>
      <ProcessingDetails>
        <Name>H18</Name>
      </ProcessingDetails>
      <PropertyData property=”p1” source=”s1”>
        <Data format=”integer”>23,17,15</Data>
      </PropertyData>
    </BulkDetails>
    <Metadata>
      <DataSourceDetails id=”s1”>
        <Name>“Properties of Aluminum Alloys… </Name>
      </DataSourceDetails>
      <PropertyDetails id=”p1”>
        <Name>Axial-Stress Fatigue Strength</Name>
        <Units name=”ksi” Description=”kip per square inch”>
          <Unit>kip</Unit>
          <Unit power=”-2”>inch</Unit>
        </Units>
      </PropertyDetails>
    </Metadata>
  </Material>
</MatML_Doc>
```



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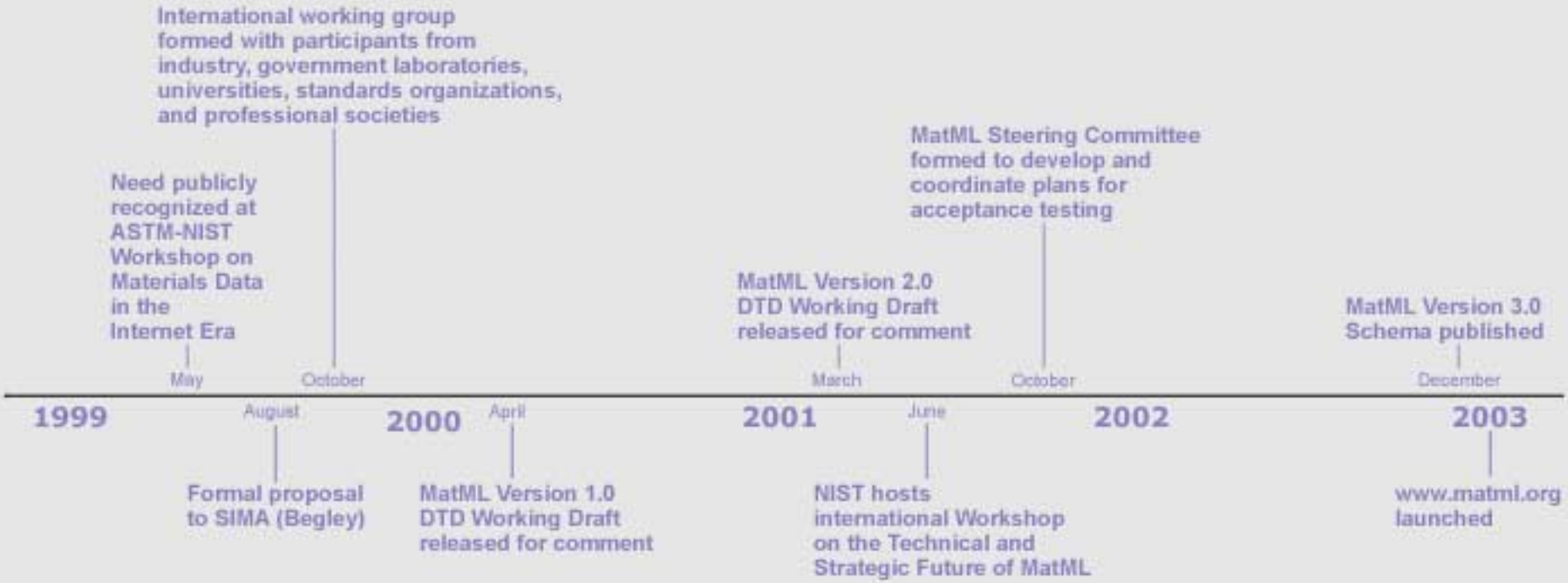
# MatML: Definition, History, Results



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# MatML: Definition, History, Results


**MatML Working Group [1999 – 2001]**

**Industry and Professional Societies**

- C. Bullough, ABB ALSTOM Power, UK
- F. Cverna, ASM International
- S. Gurke, knovel Corporation
- G. Kaufman, Aluminum Association
- T. Kipp, MSC.Software
- S. McCormick, ESM Software
- J. Phipps, William Andrew Publishing
- D. Rose, AMPTIAC
- M. Smith, CenTOR Software Corp.
- M. Stoeckle, Ford Motor Company
- M. Sullentrup, The Boeing Company

**NIST**

- E. Begley, Project Leader
- B. Boettinger, Metallurgy
- S. Dapkunas, Ceramics
- C. Handwerker, Metallurgy
- V. Karen, Ceramics
- U. Kattner, Metallurgy
- R. Munro, Ceramics
- J. Rumble, SRD
- T. Siewert, Materials Reliability
- C. Sturrock, SRD
- C. White, Building Materials

**Non-NIST Government and Academia**

- T. Baba, Nat'l Research Lab. Metrology, Japan
- C. Gibson, CINDAS, Purdue University
- K. Halada, Nat'l Inst. Materials Science, Japan
- D. Martin, Iowa State University
- J. McCarthy, Lawrence Berkeley Nat'l Lab.
- J. Michopoulos, U.S. Naval Research Lab.
- F. Moran, Atomic Weapons Establishment, UK
- P. Murray-Rust, Nottingham University, UK
- C. Newton, University of Delaware
- F. Olken, Lawrence Berkeley Nat'l Lab.
- A. Powell, Massachusetts Institute of Tech.
- D. Readey, Colorado School of Mines



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# MatML: Definition, History, Results




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# MatML: Definition, History, Results

**MatML Steering Committee [2001 – 2003]**

- G. Kaufman, Aluminum Association (retired), Chairman
- E. Begley, NIST, Lead Technical Expert
- F. Cverna, ASM International
- D. Fleming, MatWeb.com
- C. Grethlein, AMPTIAC
- C. Hammond, General Electric Company
- S. McCormick, ESM Software
- D. Mies, MSC Software
- M. Kmetz, IDES, Inc.
- M. Mitchell, NASA Marshall Space Flight Center
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- J. Pillers, Boeing Phantom Works
- J. Rossi, Westmoreland Testing and Research, Inc.
- C. Seymour, Granta Design Limited
- M. Sullentrup, Boeing Aircraft Programs




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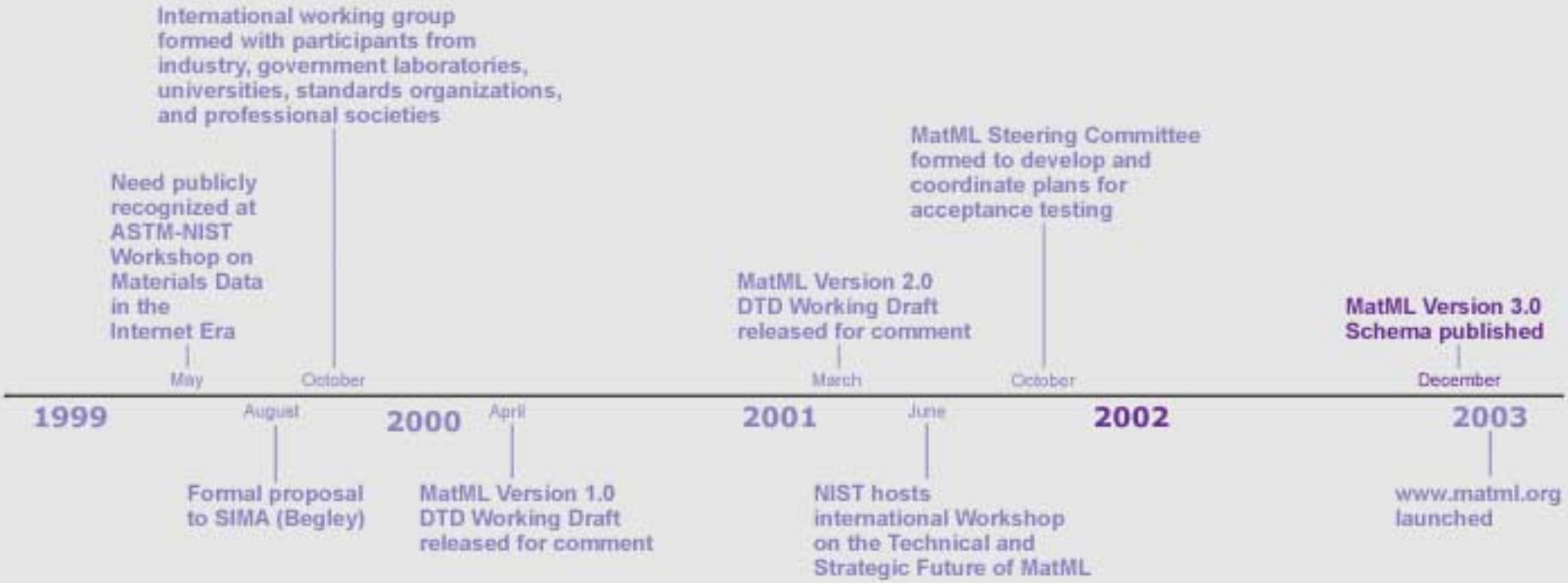
# MatML: Definition, History, Results



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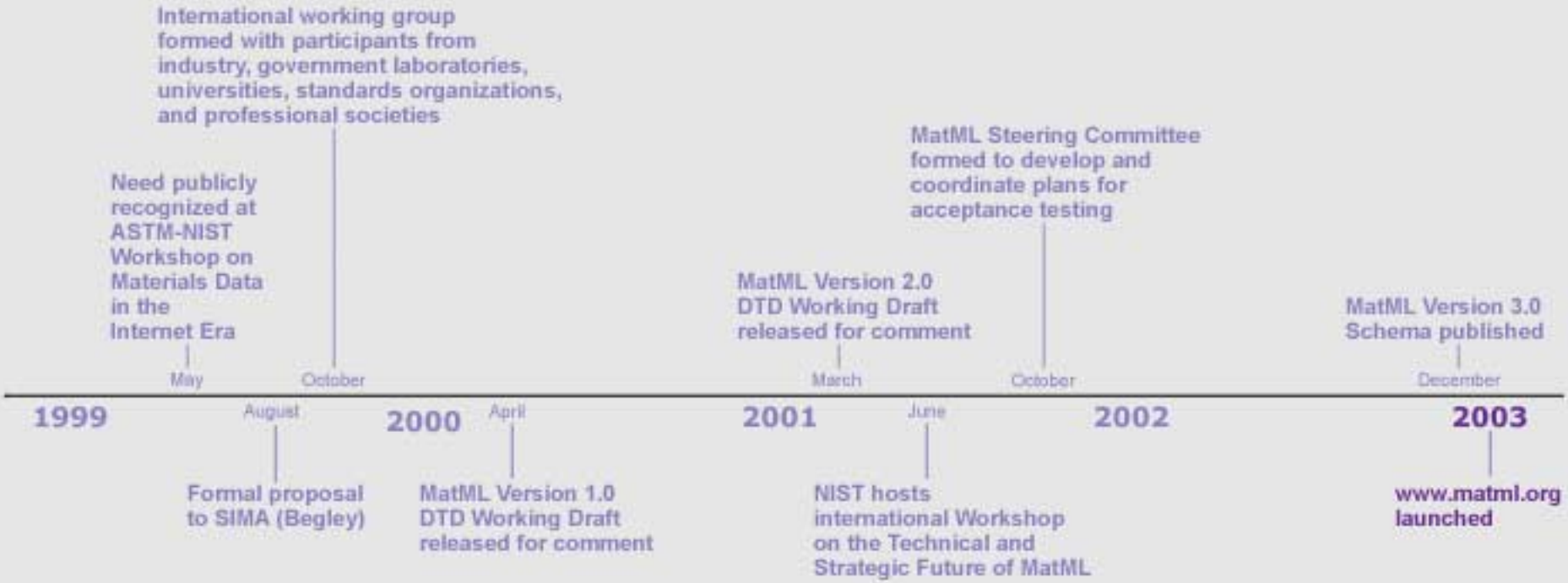
# MatML: Definition, History, Results



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# Technical: MatML Schema

```
<?xml version="1.0" encoding="UTF-8"?>
<!--
        ********************************************************************************************************************
        Title
        MatML Version 3.0 Schema

        Author
        This document was prepared by E.F. Begley (begley@nist.gov) on behalf of the MatML Working Group
        (1999-2001) and the MatML Steering Committee (2002).

        Copyrights
        This work is an official contribution of the National Institute of Standards and Technology (NIST) and is
        not subject to copyright in the United States.

        "METADATA" is a trademark of the Metadata Company. Any use of the term "metadata" in this
        document is in a descriptive sense, meaning "data about data." MatML is not in any way affiliated with
        the Metadata Company.

        ********************************************************************************************************************
        Acknowledgements
        The MatML development effort has provided deeply satisfying personal and professional challenges for
        the author. He gratefully acknowledges the contributions of his collaborators.

        Funding
                This project was funded [in part] by NIST's Systems Integration for Manufacturing Applications
                (SIMA) Program. SIMA supports NIST projects applying information technologies and
                standards-based approaches to manufacturing software integration problems.

        Project Support
                Standard Reference Data Program (SRD), NIST
                Materials Science and Engineering Laboratory (MSEL), NIST
                Building and Fire Research Laboratory (BFRL), NIST

        Technical Collaboration
                The MatML Working Group (1999-2001)
                        Members External to NIST
                                Tetsuya Baba, National Research Laboratory of Metrology, Japan
                                Chris Bullough, ABB ALSTOM Power, Leicester UK
                                Fran Cverna, ASM, International
                                Charles Gibson, Center for Information and Numerical Data Analysis and Synthesis (CINDAS)
                                Sasha Gurke, William Andrew Publishing
                                Kohmei Halada, National Research Institute for Metals, Japan
                                Gil Kaufman, Aluminum Association, Inc.
                                Tom Kipp, MSC.Software
                                David Martin, Iowa State University
                                John McCarthy, Lawrence Berkeley National Laboratory
                                Scott McCormick, ESM Software
                                John Michopoulos, United States Naval Research Laboratory (USNRL)
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                                Crystal Newton, Center for Composite Materials, University of Delaware
                                Frank Olken, Lawrence Berkeley National Laboratory
                                Jon Phipps, William Andrew Publishing
                                Adam C. Powell, Massachusetts Institute of Technology
                                Dennis Readey, Colorado School of Mines
                                David Rose, Advanced Materials and Processes Technology Information Analysis Center (AMPTIAC)
                                Martin Smith, CenTOR Software Corporation
                                Michael Stoeckle, Ford Motor Company
                                Mike Sullentrup, The Boeing Company
                        NIST Members
                                Bill Boettinger, Metallurgy Division, MSEL
```

# MatML: Definition, History, Results

## Technical: MatML Schema

A MatML document is compartmentalized into 5 major elements:

1. BulkDetails contains a description of the bulk material
2. ComponentDetails contains a description of each component of the bulk material, which is useful for complex materials systems such as composites or welds
3. Metadata contains descriptions of data found in the document
4. Graphs encodes two-dimensional graphics
5. Glossary contains definitions of terms found in the document


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# MatML: Definition, History, Results

| *BulkDetails contains description of the bulk material* | |
|---|---|
| **Tag** | **Use** |
| Name | Name of bulk material |
| Class | Class of bulk material |
| Subclass | Subclass of class |
| Specification | Specification of bulk material |
| Source | Source of bulk material |
| Form | Form of bulk material |
| ProcessingDetails | Description of processing history |
| Geometry | Description of geometry |
| Characterization | Characterization including chemical formula, chemical composition, phase composition, and dimensional details |
| PropertyData | Property data |
| Notes | Additional information |


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# MatML: Definition, History, Results

| *ComponentDetails contains description of each component of the bulk material* | |
|---|---|
| **Tag** | **Use** |
| Name | Name of component |
| Class | Class of component |
| Subclass | Subclass of component |
| Specification | Specification of component |
| Source | Source of component |
| Form | Form of component |
| ProcessingDetails | Description of processing history |
| Geometry | Description of geometry |
| Characterization | Characterization including chemical formula, chemical composition, phase composition, and dimensional details |
| PropertyData | Property data |
| AssociationDetails | Description of the relationship of the component to another component |
| Notes | Additional information |
| ComponentDetails | Description of a component within the component |


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# MatML: Definition, History, Results

*Metadata contains descriptions of the data sources, properties, measurement techniques, specimens, and parameters encoded within the MatML Document*

| Tag | Use |
|---|---|
| DataSourceDetails | Description of a data source |
| PropertyDetails | Description of a property |
| MeasurementTechniqueDetails | Description of a measurement technique |
| SpecimenDetails | Description of a specimen |
| ParameterDetails | Description of a parameter |


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# MatML: Definition, History, Results

| *Graphs describes two-dimensional graphics and allows for three types of graphical objects: vector graphics shapes, images, and text* | |
|---|---|
| **Tag** | **Use** |
| **W3C's Scalable Vector Graphics markup language (SVG)** | **See http://www.w3.org/TR/SVG/** |

# MatML: Definition, History, Results

| *Glossary contains definitions of terms found in the MatML document* | |
|---|---|
| **Tags** | **Use** |
| **Name** | **Name of term** |
| **Definition** | **Definition of term** |
| **Abbreviation** | **Abbreviation(s) of term** |
| **Synonym** | **Synonym(s) of term** |
| **Notes** | **Additional information pertinent to the term** |



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# MatML: Definition, History, Results

| Tagset for MatML Version 3.0 Schema | | |
|---|---|---|
| Associate | Geometry | PropertyDetails |
| AssociationDetails | Glossary | Qualifier |
| BulkDetails | Graphs | Relationship |
| Characterization | Material | Result |
| ChemicalComposition | MatML_Doc | Shape |
| Class | MeasurementTechniqueDetails | Source |
| ComponentDetails | Metadata | Specification |
| Compound | Name | SpecimenDetails |
| Concentration | Notes | Subclass |
| Data | Orientation | Symbol |
| DataSourceDetails | ParameterDetails | Uncertainty |
| DimensionalDetails | ParameterValue | Unit |
| Dimensions | PhaseComposition | Unitless |
| Element | ProcessingDetails | Units |
| Formula | PropertyData | Value |


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# Technical: Catalog of Examples

```
<?xml version="1.0" encoding="UTF-8"?>
<!--
        ********************************************************************************************************************
        MatML Version 3.0 Schema Example 1 - Structural Ceramic from an Online Materials Database
        Prepared by - E.F. Begley, NIST
        Source - NIST WebSCD, http://www.ceramics.nist.gov/srd/scd/Z00363.htm, R.G. Munro and E.F. Begley,
        January 2002
        ********************************************************************************************************************
-->
<MatML_Doc xmlns:xsi="http://www.w3.org/2000/10/XMLSchema-instance" xsi:noNamespaceSchemaLocation="matml.xsd">
        <Material>
                <BulkDetails>
                        <Name>silicon nitride</Name>
                        <Class>ceramic</Class>
                        <Subclass>nitride</Subclass>
                        <Specification>NCX-5102</Specification>
                        <Source>Saint-Gobain/Norton Industrial Ceramics</Source>
                        <Form>bar</Form>
                        <ProcessingDetails>
                                <Name>hot isostatic pressing</Name>
                                <Notes>
                                        "The material produced is designated NCX-5102 and consists of a silicon nitride-4% yttria composition
                                        that is densified by glass-encapsulation HIPing. ... Large-scale batches (30 kg) of Si3N4-4% Y2O3
                                        powder were milled in water, and the slurry was used to cast hundreds of tensile rods. The starting Si3N4
                                        powder (Ube) was derived from a dimmide process. ... The net-shape-formed bars were HIPed using
                                        glass encapsulation (ASEA Cerma AB, Robertsford, Sweden). The HIP process was optimized using
                                        pressure, time and temperatures to assure full densification and development of an elongated
                                        microstructure for desired fracture toughness..."
                                </Notes>
                        </ProcessingDetails>
                        <Characterization>
                                <Formula>Si3N4·4wt%Y2O3</Formula>
                                <ChemicalComposition>
                                        <Compound>
                                                <Element>
                                                        <Symbol subscript="3">Si</Symbol>
                                                </Element>
                                                <Element>
                                                        <Symbol subscript="4">N</Symbol>
                                                </Element>
                                        </Compound>
                                        <Compound>
                                                <Element>
                                                        <Symbol subscript="2">Y</Symbol>
                                                </Element>
                                                <Element>
                                                        <Symbol subscript="3">O</Symbol>
                                                </Element>
                                                <Concentration>
                                                        <Value format="integer">4</Value>
                                                        <Units description="mass fraction">
                                                                <Unit>%</Unit>
                                                        </Units>
                                                </Concentration>
                                        </Compound>
                                </ChemicalComposition>
                        </Characterization>
                        <PropertyData property="pr1" technique="mt1" source="ds1">
                                <Data format="integer">972,561</Data>
                                <ParameterValue parameter="pa1" format="integer">23,1370</ParameterValue>
                        </PropertyData>
```



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## Technical: Catalog of Examples

See NISTIR 6939, pages 35 – 43 for fully worked examples:

1. Structural ceramic from an online materials database
2. Aluminum alloy from a printed handbook
3. Steel with TiC coating from a journal article


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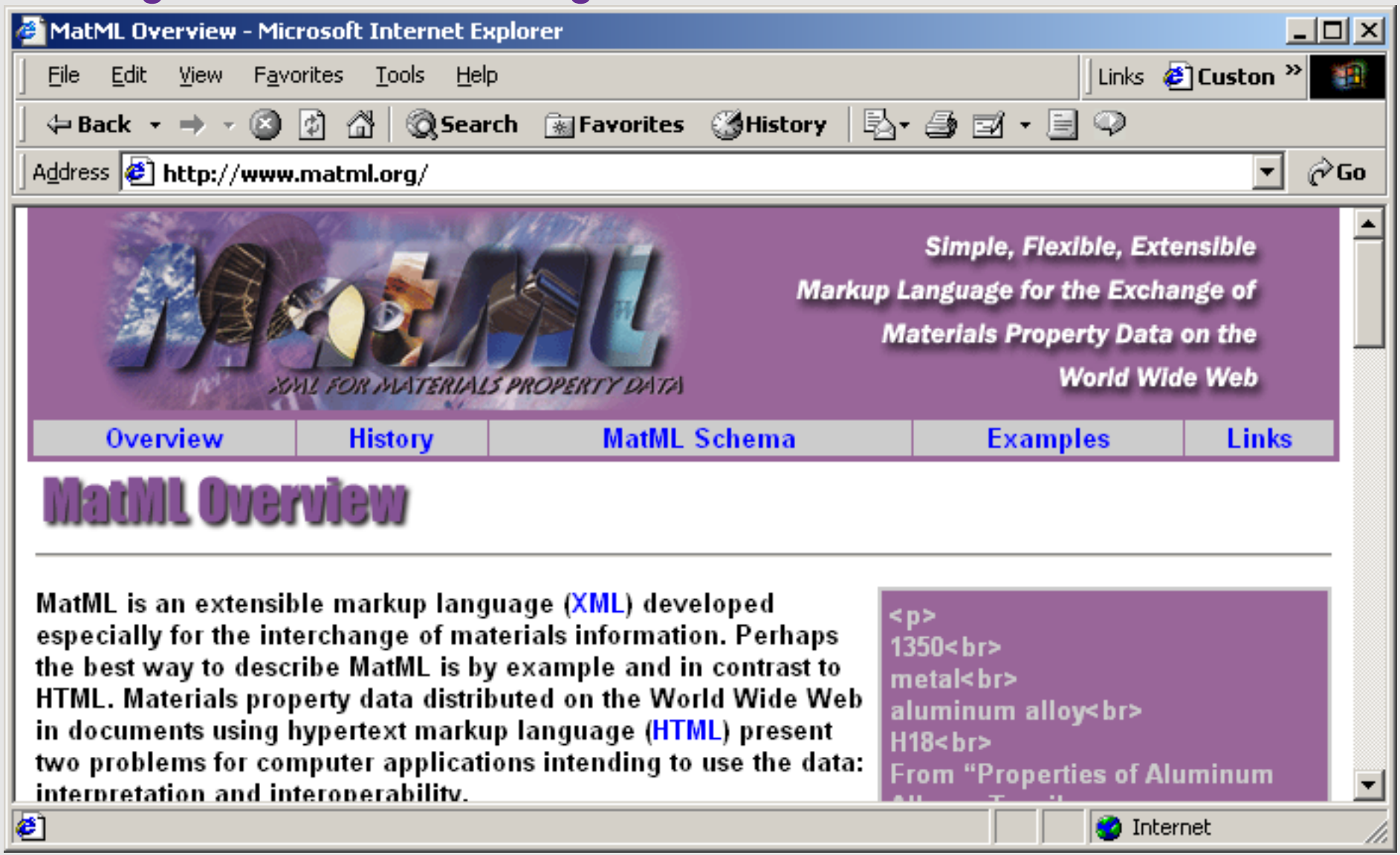
# MatML: Definition, History, Results

## Strategic: www.matml.org



# MatML: Definition, History, Results

## Strategic: Testing and Evaluation

- Finite element modeling markup language (femML): femML (www.istos.org/femML/) uses MatML via namespace for managing materials data within femML documents.
- Application to MatWeb Materials Information Downloads: MatWeb (www.matweb.com) has a trial export format for MatWeb in place, and is fully committed to MatML as an option for distributing materials information from the site.
- Granta Design Application of MatML: Granta Design (www.grantadesign.com) is working on a trial application with which users might download materials information in MatML format using Granta Design software.
- Granta Design Application of MatML for NIST MSEL: On contract from the NIST Materials Science and Engineering Laboratory, Granta Design is working on the use of MatML for the distribution of materials information by MSEL's Metallurgy Division.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# MatML: Definition, History, Results

## Strategic: Testing and Evaluation

- Laboratory Test Equipment Application of MatML: A Test Data Exchange Working Group has been established to evaluate the reporting of materials information from laboratory test equipment to lab customers using MatML. Westmoreland Mechanical Testing & Research (www.wmtr.com) will utilize sample customer orders requesting data in MatML as the output format.
- NASA MSFC Utilization of MatML: NASA Marshall Space Flight Center (www1.msfc.nasa.gov/) has funded a program with Centor Software (www.centor.com) that includes the evaluation of MatML for the exchange materials information among NASA sites.
- ASM/MSC Application of MatML for Publication Development: ASM International (www.asm-intl.org) and MSC Software (www.mscsoftware.com) are evaluating the use of MatML to handle the transmission of materials information from ASM to MSC for the development of new ASM publications.


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# MatML: Definition, History, Results

## Strategic: Early Stage of Consideration

- General Electric Corporation: General Electric (Schenectady) is considering the application of MatML for the exchange of materials information within that organization.
- MIL-HDBK-5, 17: The producers of the military handbooks that cover materials information, commonly referred to as MIL-HDBK-5 and MIL-HDBK-17, have expressed interest in the possible use of MatML in their exchange of materials information.
- Building & Construction Industries; Cement & Concrete: American Concrete Institute (http://www.aci-int.org/general/home.asp) experts are discussing the possible use of MatML for the exchange of materials information for B&C applications of these products.
- Test Equipment Manufacturers: Discussions have been initiated with several test equipment manufacturers (Instron and MTS Systems Corp.) on possible applications of MatML in their test equipment data output software.


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# MatML: Definition, History, Results

## Strategic: Early Stage of Consideration

- ANSYS: The developers of ANSYS have expressed some interest in the use of MatML for the interchange of materials information.
- SETAC/Life-Cycle Assessment Advisory Group: MatML has been proposed as a tool for the exchange of materials information by the Society of Environmental Toxicology and Chemistry Life-Cycle Assessment Advisory Group. Consideration will be given to submitting a paper at a future SETAC/Europe Conference, where that application may be further explored.
- Swedish Industrial Consortium: The Swedish Industrial Consortium is considering the possible application of MatML for the distribution of materials information from their website.


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# MatML: Definition, History, Results

## Recent and Upcoming Events

- **MatML registered and reposited at xml.org**
  **(xml.org works to minimize overlap and duplication in XML languages and XML standard initiatives by providing public access to XML information and XML Schemas)**
- **OASIS MatML Technical Committee established (initiated by NIST, NASA, and Boeing)**
  **(OASIS, Organization for the Advancement of Structured Information Standards, is a not-for-profit, global consortium that drives the development, convergence and adoption of e-business standards. See: http://www.oasis-open.org)**
- **MatML's future development handed off from NIST to Industry Development Working Group chaired by Doug Fleming of MatWeb.com (doug.fleming@matls.com) on 06 May 2003.**
- **Prototype MatML Editor Development Project to be initiated this summer (Sponsored by MSEL Center for Theoretical and Computational Materials Science and BFRL)**
- **Neutral MatML Industry Management Group being formed to replace NIST-sponsored MatML Steering Committee (meeting planned for 05-06 June 2003)**